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# Energy transport and correlation between two attractors connected by Fermi-Pasta-Ulam chain

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## Abstract

We study numerically time evolution of a system which consists of two attractors connected by Fermi-Pasta-Ulam (FPU) chain. It is found that after sufficiently long time there exits self-consistent large scale structure in the system. The wavelet transform is used to separate the modes in different scales. We found that the nonlinear long wavelength mode propagating along the chain assists the energy transport. Further, all points in the system are found to be correlated. Our results explain satisfactorily why the chaotic behaviour is not enough to ensure the Fourier heat law and the thermal conductivity diverges as it is found recently by Lepri *et al* (PRL **78**, 1897(1997).).

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The finding of Fermi-Pasta-Ulam [1] in 1955, i.e. the absence of the energy equipartition in a system of coupled nonlinear oscillators, becomes one of the cornerstones in the modern statistical mechanics [2,3]. It stimulated the study of nonlinear dynamics and chaos.

Since the first numerical experiment of FPU , many works have been done on one-dimensional anharmonic oscillators to study various problems related to irreversiblie statistical mechanics [2]. In addition to many applications of FPU model to study the relation between the stochastic motions and thermodynamics properties [4,5], the FPU model is used very recently to study another important problem in nonequilibrium system by Lepri *et al* [6] (thereafter refereed to as LLP), namely the Fourier heat conduction law in insulating solids. In LLP's study, two Nosé-Hoover "thermostats" [7,8] were put on the first and last particles of FPU-$\beta$ model (FPU model with quartic potential) keeping the temperature at $T_+$ and $T_-$, respectively. The two ends of the chain are fixed. After a certain transient time, the nonequilibrium stationary state sets in and a nonlinear shape of temperature profile is formed. The temperature is found to have scaling relation $T_l = T(l/N)$, here $N$ is the number of the particles. The heat flux is found to be $N^{1/2}$. Therefore, the thermal conductivity $\kappa$ is divergent approximately with the length of the chain as $N^{1/2}$, and the Fourier heat law is not justified. Compared with that case of the ding-a-ling model [9], where the heat transport obeys the Fourier heat law, LLP concluded that the chaotic behaviour is not sufficient to ensure the Fourier heat law.

Although it is commonly believed that the anharmonicity or the nonlinear interaction leads to the scattering of phonons, the mechanism leading to the divergence of the thermal conductivity in FPU model and other similar nonlinear oscillator chains is still lacking. In fact, it is a very general problem in the field of statistical physics to understand the origin of the irreversibility and its compatibility with the time reversible deterministic microscopic dynamics.

In this paper, concentrating on time evolution of system used by LLP, we would like to clarify the mechanism behind the divergence of the thermal conductivity. The equations of motion of the two particles keeping at the "thermostats" are determined by,

$$\begin{aligned} \ddot{x}_1 &= -\zeta_+ \dot{x}_1 + f_1 - f_2, \\ \ddot{x}_N &= -\zeta_- \dot{x}_N + f_N - f_{N+1}, \\ \dot{\zeta}_+ &= \frac{\dot{x}_1^2}{T_+} - 1, \qquad \dot{\zeta}_- = \frac{\dot{x}_N^2}{T_-} - 1. \end{aligned} \tag{1}$$

The equation of motion for the central particles is,

$$\ddot{x}_i = f_i - f_{i+1}, \qquad i = 2, \ldots, N-1, \tag{2}$$

where $f_i = -V'(x_{i-1} - x_i)$ is the force acting on the particle, $V(x) = x^2/2 + \beta x^4/4$. $x_0 = 0$ and $x_{N+1} = 0$. It is obvious, the dynamical equations are invariant under time reversal combined with the change $p_i \to -p_i$.

As an alternative, the coupling of a chain of N particles to thermal reservoirs can be realized by numerical random generators [10]. In this case at each time step, the velocities of the first and last particles are determined by sampling randomly from the Maxwellian distribution corresponding to reservoirs temperatures. This approach allows one to achieve quickly steady state for time-averaged temperature profile for sufficiently long chain to study dependence of thermal conductivity as a function of the system size $N$. In its turn, Nosé-Hoover

"thermostats" were proposed specially as the extension of molecular dynamics methods to treat the problems relating to the question [2,7]: can statistical mechanics be derived from the underlying dynamics?

It has been shown that the canonical distribution with given temperature can be generated with smooth, deterministic and time reversible trajectories. However, simple numerical examples given in [8] illustrate that a single oscillator which is used usually for the boundary "thermostat" in the equations (1) can not be sufficiently chaotic to yield the canonical distribution from a single initial condition. Really, for the parameter we chosen, $T_+ = 152, T_- = 24$ (the same as LLP used), and $\beta = 0.5$, the time evolution of the two ""thermostats" are not sufficiently random. There are some periodic-like structures in the phase space (see Fig.1). These two "thermostats" are not really thermostats, instead they are attractors covering only part of the phase space. It is not quite clear that even large system including these two subsystems as the "boundary conditions" will behave quite randomly.

In fact we are dealing with long but finite system driven by two attractors which are connected by FPU $\beta$ chain. Energy balance is fixed by the two "thermostats" only and dissipation is absent. This means that a memory about some excitations generated once in this system may not disappear during thermalization process.

The time evolution of the displacement at initial time period ($10^2$ time units) as well as after long enough time (the same time period, but after $10^4$ time units) are shown in Fig. 1c,d respectively. It is evidently that there are some kind of nonlinear excitations propagating inside the system, which does not disappear even after long time. A combination of the parameters of the chain and "thermostats" leads to some mesoscopic structures.

We tested that after sufficiently long averaging this structure is not reflected directly on the "temperature" profile. (Temperature is defined as the twice of the kinetic energy). Namely, the temperature profile is smooth and exactly has the scaling $T_l = T(l/N)$ as observed by LLP. However, at least two different kinds of regular motion alive in the system at sufficiently long time. There are quasi-soliton nonlinear excitations performing non-diffusive energy transport between two boundary attractors and longwave stationary eigenmodes of displacements along the chain.

First ones are nonlinear excitations which move back and forth and scattered by the boundaries. Their presence is the main reason for the seemly singularity of the temperature profile near the boundary. As an independent test, we initialized the displacement by a localized excitation and let it propagate along the chain (Fig.2a). We calculate the "temperature" profile caused by the propagation of this excitation (Fig. 2b). It shows specific structure near the boundary as displayed in the temperature profile in LLP.

The second kind of motion can be compared to that of an effective harmonic oscillators with rescaled frequencies and modulated amplitudes existing at different time scales. If we take enough long time for the simulation, then the oscillations of very long period are observable. Besides, the time taken to reach the same level of thermalization essentially grows with the chain length $N$. Strictly speaking, this makes impossible the simulation of the thermodynamic limit.

Nevertheless, the thermalization-like process is realized in the nonequilibrium stationary state. Fig. 3. shows the probability distribution function of the velocity of the particles near the boundary and that inside the chain far from the boundary. They are really good

Gaussian function, with the widths proportional to the averaged temperatures at the same points.

Although this nonlinear chain is stochastic, it is not stochastic enough to be a purely random system. Let us plot the time-evolution of the displacement. The particular plot in Fig. 4. shows the system having 64 particles. The equation of motion have been integrated through a standard fifth-order Runge-Kutta routine, using double precision with a maximal step equal to $10^{-3}$. The time in Fig 4a begins after a transient period of $10^8$ steps and changes from 0 to 163.84 time units. The color shows the displacements from most negative ("cold" colors) to most positive ("hot") values. Qualitatively the same figures were obtained for other chains (from 32 till 1024 particles). It has been checked also for the structures obtained after very long time transient periods as well as much longer time inteval of observation were used (up to 1638.4 units).

Strongly pronounced periodic structure in this picture corresponds to the longest oscillation visible during the demonstrating time period[1]. It shades other waves in system. Presence of the excitations with different scale makes it impossible to separate them in ordinary Fourier transform approach. However, it can be done with help of more sophisticated wavelet transform, which allows us to separate the excitations in different scales naturally [12]. To filtrate the modes a standard Daubechies wavelets of 20 order DAUB20 have been used [13]. The wavelet transform over time has been performed for every particle and truncation is made over first 0.39% wavelet coefficients.

The filtration gives clear picture of the long wavelength motion, shown in Fig. 4b. Fig. 4c displays mesoscopic structure which remains after subtraction of the above large-scale structure from the complete one shown in Fig 4a. Many short wave excitations moving left and right without energy loss are seen clearly. They are found to be responsible for instant local heat flux $J_i(t)$ in the system. Last value has the interpretation of the flow of potential energy from the $i$th to its neighboring particle and can be written in the form

$$J_i(t) = \dot{x}_i f_{i+1}. \tag{3}$$

The time-space distribution for the $J_i(t)$ value is displayed explicitly (without wavelet transform) in Fig. 4d and should be compared with mesoscopic structure in Fig.4c.

The regular energy transport along the chain generates long-time correlations between displacements in the system. It is reflected by the correlation functions

$$C_{ij}(t') = \langle x_i(t) x_j(t+t') \rangle \tag{4}$$

Fig.5a shows the autocorrelation function $C_{ii}$ (each of them is normalized on its maximum). It is seen from this picture that the $C_{11}$ and $C_{NN}$ have a form qualitatively close to that of independent chaotic attractors. The quasi-periodic correlations inside the chain are also visible. In addition, an interaction between particles leads to strong correlations between main periods of motion for different points, including the particles at both ends. This is

[1]Note that the period of this structure is found to be proportional to $N$, whereas that of soliton in FPU model is proportional to $N^{5/2}$.

readily depicted by $C_{1N}$ shown in Fig. 5b. This plot is quite essential. It tells us that due to interaction via the chain some regular correlation shows up even between the two particles which are supposed to be kept at the "thermostats".

In conclusion, formation of attracting large-scale structure as well as the nonlinear excitation of propagating waves are the main courses which make the energy transport in such a system *impossible* to obey the Fourier heat law. The results given here suggest that, in order to have energy transport obey the Fourier heat law, we need to add some ingredients such as the periodic external potential [14], which is analogous to the lattice, to inhibit such kind of structure and long wavelength propagating modes.

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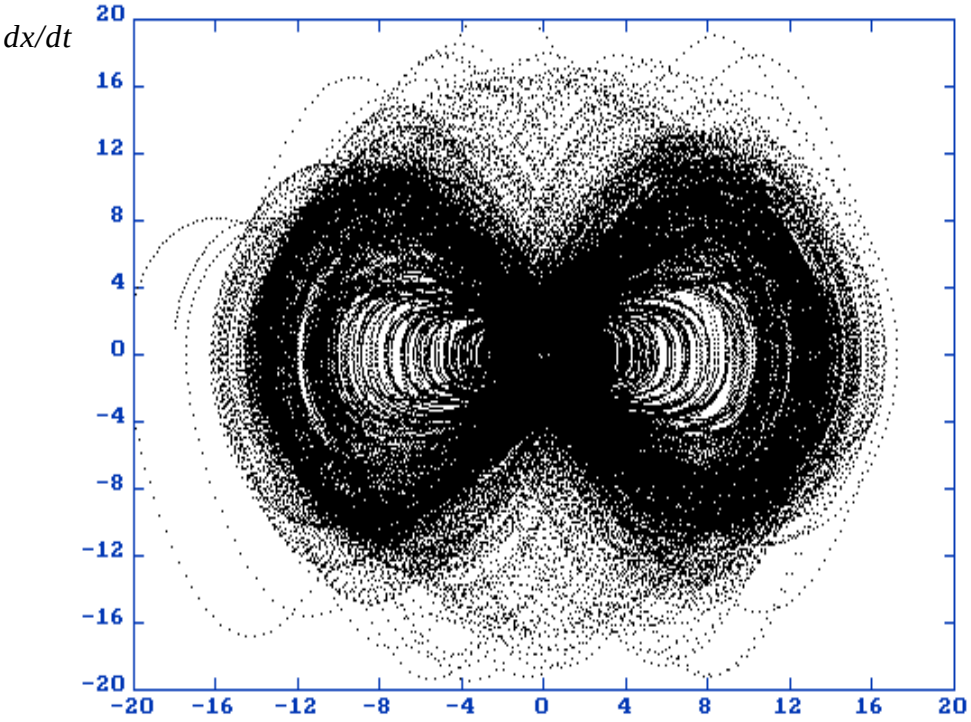
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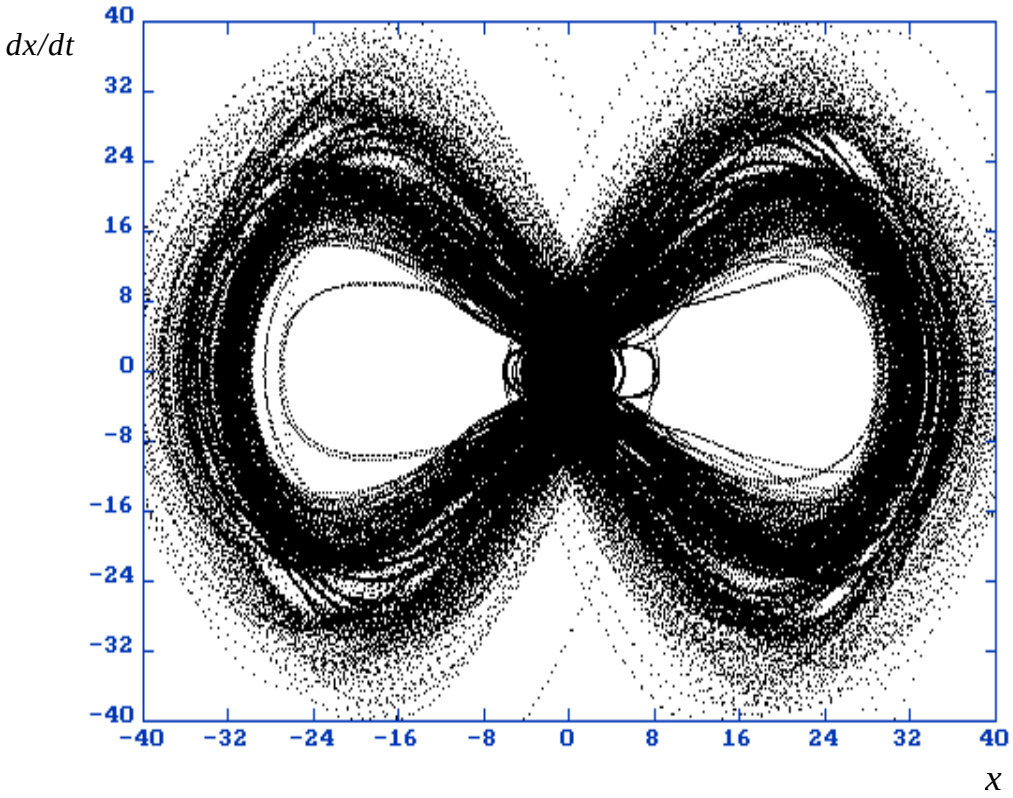
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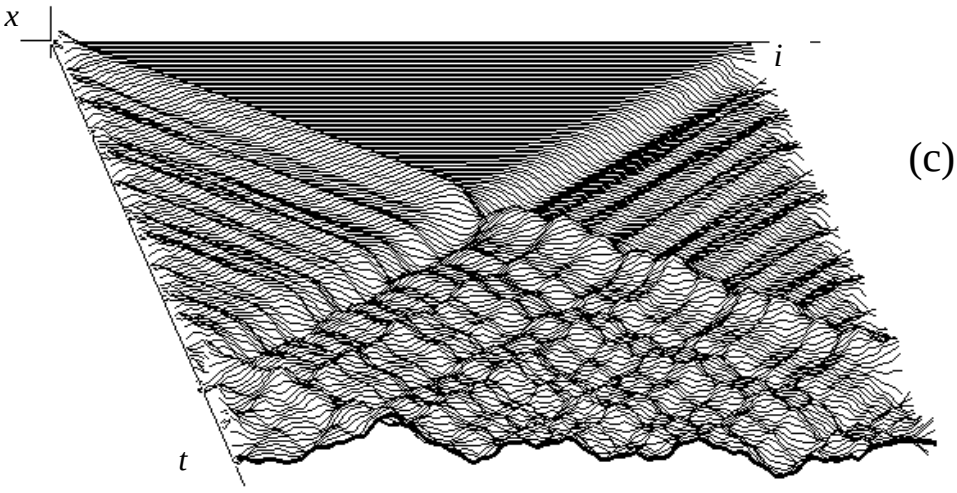


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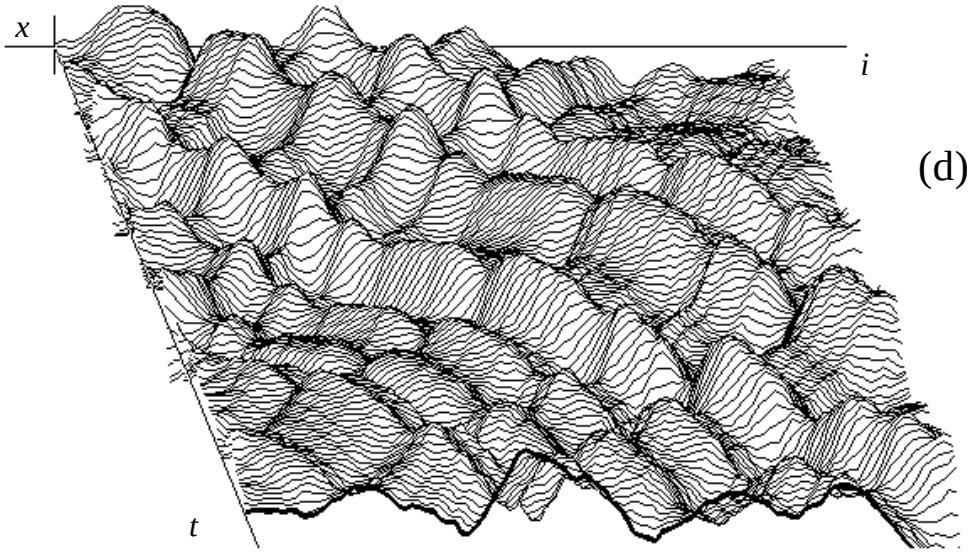


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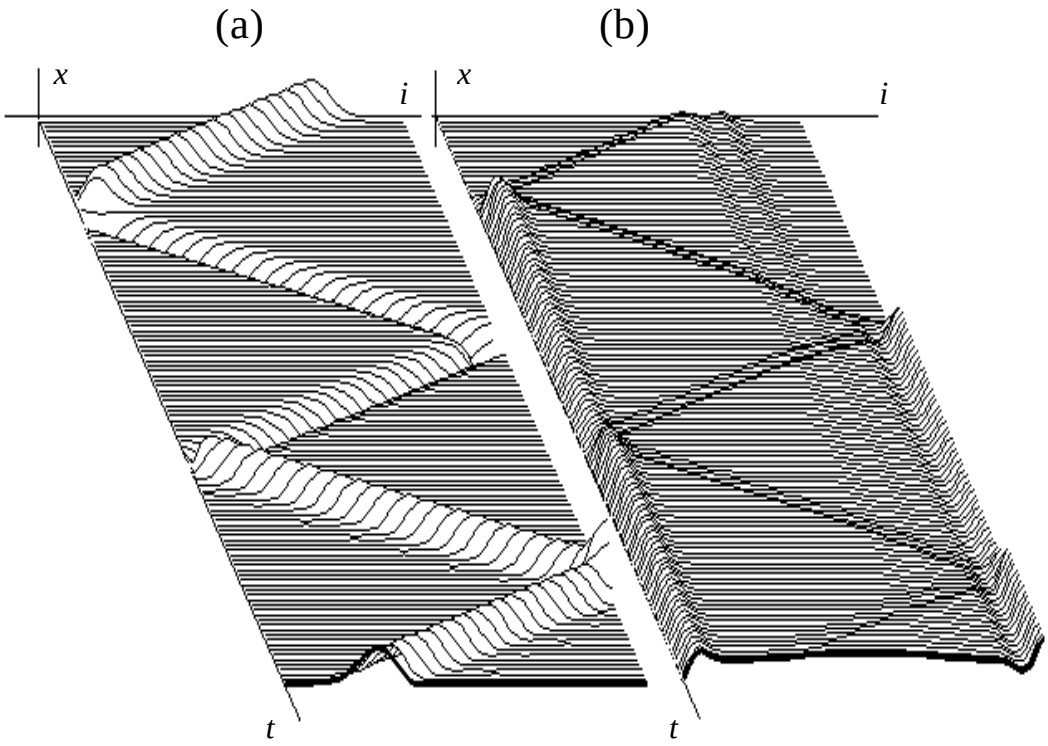
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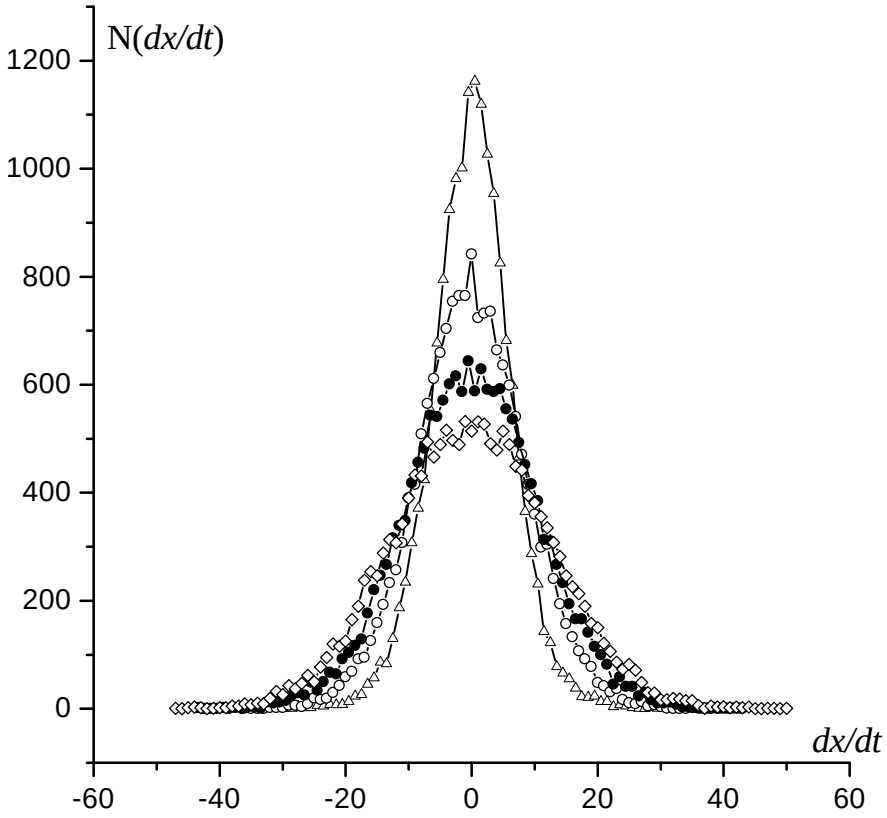
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